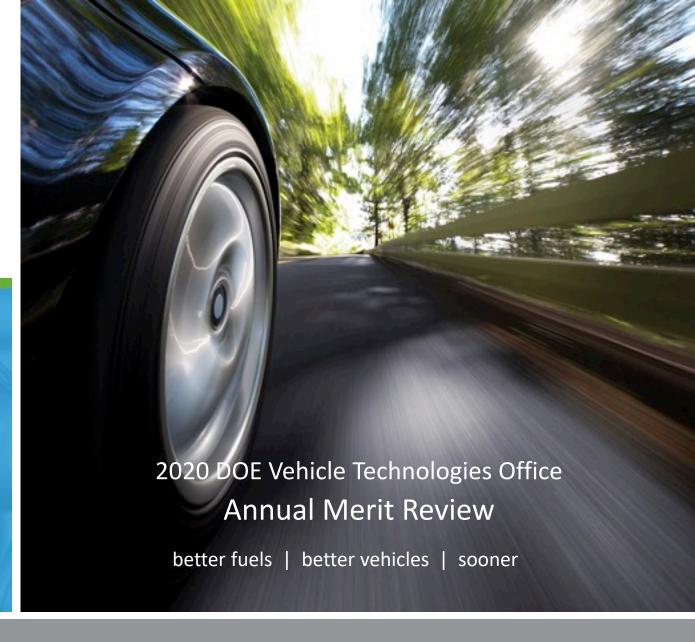


Multi-Mode Operation in Gasoline Direct-Injection Engines: Fuel-Property Effects and Approaches to Expand the Advanced Compression-Ignition Range

Toby Rockstroh (PI), Ashish Shah, Johannes Rohwer, ANL Riccardo Scarcelli (PI), Sayop Kim, ANL K. Dean Edwards (PI), ORNL

3 June 2020 Project # FT071



Overview



Projects, Timeline and Budgets

Task	FY18	FY19	FY20	FY21
MM MCE simulations (Edwards, ORNL)	(\$90k SI)			
MM/ACI sensitivity simulations (G.5.5 Edwards, ORNL)	\$75k	\$200k	\$350k	
Multi-mode SI/ACI: stratification/fuel/dilute. interactions (E.1.2.6 Curran, ORNL)	\$315k	\$222k		
Fuel Properties which Enhance Multi-Mode ACI/SI Engine Operation (E.1.2.5, Rockstroh, ANL)	\$315k	\$245k	\$300k	
Multi-mode ACI/SI Single-Cylinder GDI Engine Simulations (G.1.1.1 Scarcelli, ANL)		\$175k	\$175k	

Barriers

- 2020/2025 Stretch Efficiency Goals for downsized boosted engines
- Determine the factors limiting range of LTC and develop methods for extending the limits
- Understanding impact of likely future fuels on LTC

Partners

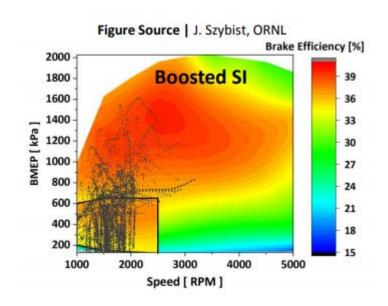
- Co-Optima program includes research funded by 2 DOE Offices at 9 National Laboratories, 20+ universities, and 1 OEM with insight from external advisory board and 80+ stakeholders
- Task specific collaborations include:
 - Other National Laboratories (e.g., LLNL, PNNL)
 - Universities (e.g., UConn)
 - Industry stakeholders (GM, Ford)
 - Software vendors (Convergent Science)

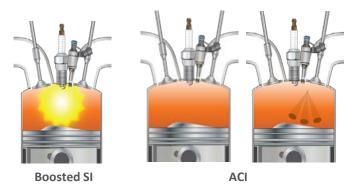
Relevance



- Co-Optima effort to identify advanced fuel properties for advanced high efficiency combustion strategies.
- Light-duty Multimode (MM) engine operation offers practical near-term fuel economy gains over significant operating map
- MM operation consists of low-load advanced compression ignition (ACI) and high-load boosted SI
 - ACI operating range combustion and control strategy challenges
 - Strategies needed to enable SI/SACI transition
 - Maintain high-load boosted SI operation

Utilize engine experiments and high-fidelity CFD modeling approaches to characterize fuel property effects and operating strategies to enhance MM engine operation



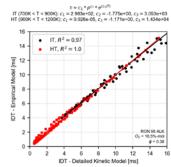


Overall Technical Approach



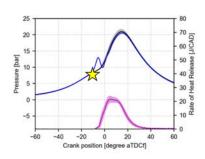
E.1.2.5 Fuel properties for MM (ANL)





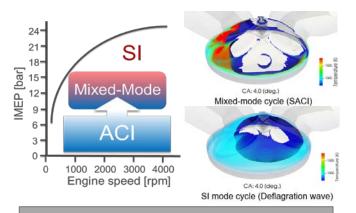
Utilize static autoignition data to define control scheme to estimate SOC for ACI



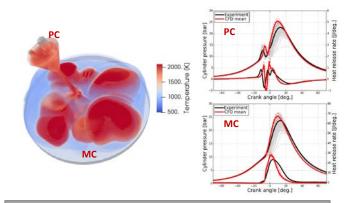


Assess pre-chamber ignition to enhance and enable ACI combustion control

G.1.1.1 MM SCE simulations (ANL)

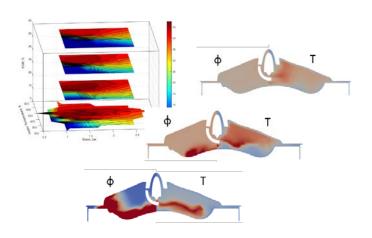


Model transition from ACI to SI and evaluate the impact of fuel properties



Model impact of pre-chamber on MM operation with focus on fuel properties

G.5.5 MM sensitivity simulations (ORNL)



Develop flexible CFD engine model to characterize fuel behavior under boosted SI and ACI operation

Milestones



Date	Lab, PI	Milestone	Status
FY2019 – Q3	ORNL, Edwards	Use LD CFD model to evaluate impact of fuel and operational parameters on MM strategies	MET
FY2019 – Q4	ANL, Rockstroh	Identify fuel autoignition performance parameters to enable SI/ACI multi-mode operation	MET
FY2019 – Q4	ORNL, Curran	Complete boundary-limit MM study across range of fuels	MET
FY2019 – Q4	ANL, Scarcelli	Explore transition strategies between ACI and SI modes	MET
FY2020 – Q2	ANL, Scarcelli	Ignition-assisted ACI operation simulated and validated	Moved to Q3*
FY2020 – Q2	ANL - Rockstroh	Preliminary evaluation of fuel combustion characteristics using a pre-chamber	Moved to Q3*
FY2020 – Q4	ANL, Scarcelli	Optimum fuel properties identified for pre-chamber assisted MM operation	On track
FY2020 – Q4	ANL – Rockstroh	Identify fuel autoignition performance parameters that enable pre-chamber assisted compression ignition operation	On track
FY2020 – Q4	ORNL, Edwards	Perform initial analysis of sensitivity to key fuel properties	On track

^{*} Delayed as a result of COVID-19 lab shutdown

Technical Approach – Project specific



E.1.2.5 Fuel properties for MM (ANL)

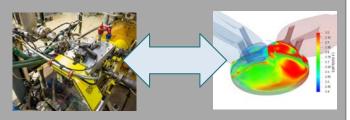
- ACI experiments on a single-cylinder GDI engine with Co-Optima core fuels
 - Compression ratio (CR) range of 11.3 15.3:1
 - Intake T, λ, load sweep
 - Intake boost pressure to control combustion phasing of 12 dATDC
- Correlating constant volume autoignition delay to engine conditions
 - Develop ignition delay map at enginerelevant thermodynamic conditions using chemical kinetic modeling
 - Capture compression history using the LW integral

$$\frac{(x)}{(x)_c} = \int_{t=0}^{t=t_i} \frac{1}{\tau} dt = 1.0$$

- Commission a prototype active prechamber ignition system*
 - Assess ACI operation and dilution tolerance using Co-Optima core fuels
 - Develop GT-Power model for detailed analysis

G.1.1.1 MM SCE simulations (ANL)

- MM CFD simulations of ANL singlecylinder engine
 - Compression ratio range of 11.3 15.3
 - 1500 RPM
 - Operating parameter sweeps:
 - Intake T, λ, load
 - Experimental data for validation



- Simulation efforts using Co-Optima core and HP fuels
 - Initial number of core fuels evaluated (ALK, E30) limited by availability of reduced kinetics for CFD simulations
 - Future directions look at PRF, TPRF, 4component BOBs, blended with alcohols (ethanol, methanol, etc.)

G.5.5 MM sensitivity simulations (ORNL)

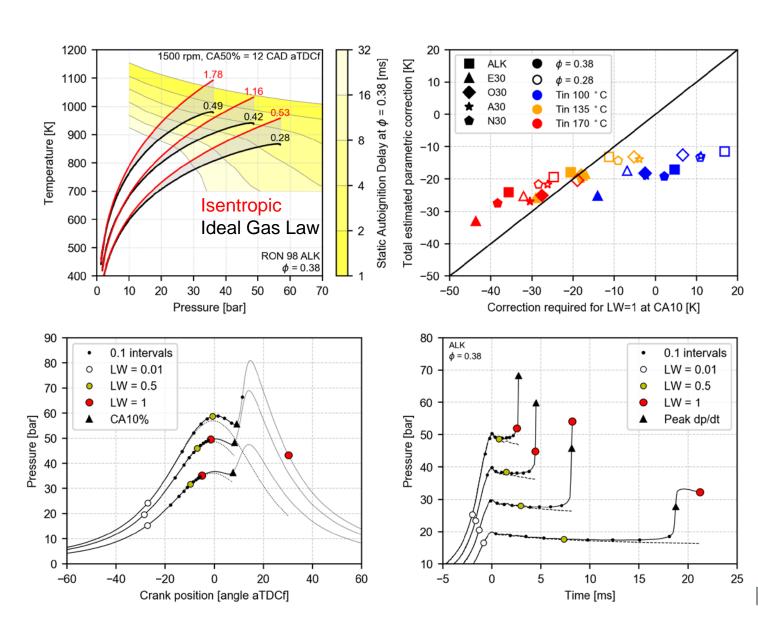
- Flexible CFD engine model allowing rapid exploration of large parameter space with 1000s of multi-cycle simulations
 - Sparse-grid sampling of parameter space with directed refinement in areas of interest (high sensitivity, good performance, etc.)
 - Results can be used to develop low-order models for faster exploration
- Engine architecture suitable for boosted SI operation at high load and ACI at low load
 - Based on Ford 1.6-L GDI
 - Maintain SI piston shapes (but modified for CR) and injector
 - Core E30 fuel surrogate and reduced mechanism
- CFD engine model to fully explore ACI parameter space
 - Intake preparation: P-T-φ-EGR%
 - Charge stratification: HCCI -> PPCI -> MCCI
 - Engine geometry: variable CR
 - Fuel properties: E30 core fuel with parameterized thermo-physical properties (HoV, vapor pressure, etc.)

^{*} Delayed as a result of COVID-19 lab shutdown

Technical Accomplishments – E.1.2.5, Rockstroh, ANL **Fuel Properties for MM - Estimating SOC**

Objective: Estimate SOC using the autoignition P-T framework

- Calculate Livengood-Wu (LW) integral for ACI compression trajectories on ignition delay map – not consistent with SOC.
- Apply cylinder temperature correction to account for heat losses, residuals and correction required for LW=1.
- Analyze LW history during compression process in the engine – cylinder conditions confounded by thermal and mixture stratification.
- RCM compression homogenous adiabatic core – constant compressed volume (PI: Scott Goldsborough).



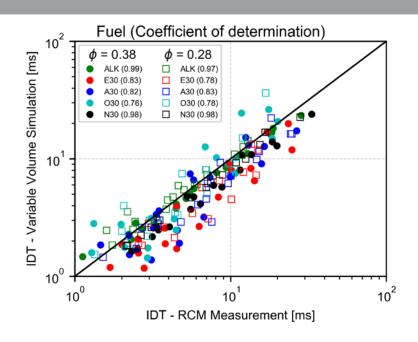
Technical Accomplishments – E.1.2.5, Rockstroh, ANL Fuel Properties for MM - Estimating SOC

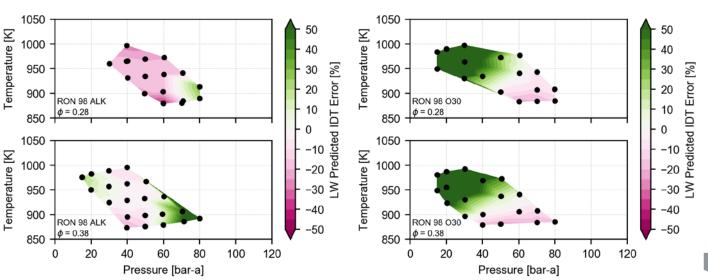


Objective: Estimate SOC using the autoignition P-T framework

- Validate ignition delay simulation against RCM measurements for two equivalence ratios and range compressed conditions.
- Considerable scatter ALK fuel good agreement across PT space – O30 limited agreement.
- Quantify the effect of difference in fuel to fuel kinetic model performance on the LW integral method using RCM measurements.
- Despite good ignition delay model performance for ALK – considerable LW error at high pressure and intermediate temperature.
- O30 significant LW prediction error.

Seemingly minor inaccuracies in kinetic model outputs can have significant influence on SOC prediction using the LW method



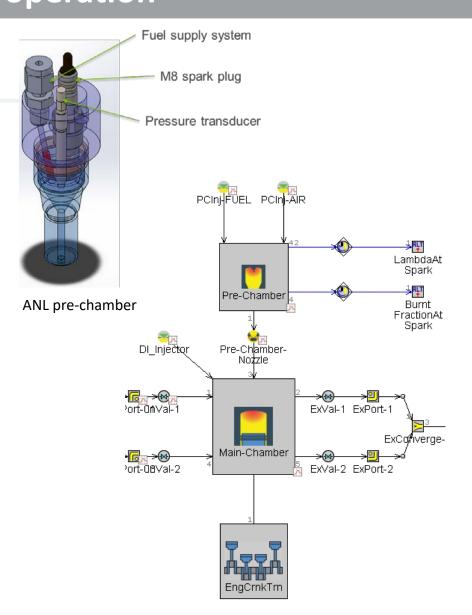


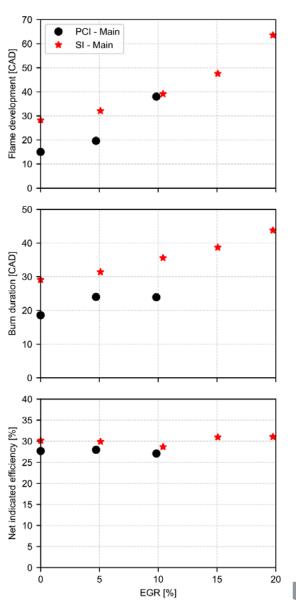
Technical Accomplishments – E.1.2.5, Rockstroh, ANL Pre-chamber assisted MM operation



Objective: Implement a pre-chamber ignition system for MM operation

- Commissioning of a pre-chamber ignition system and GT-Power model.
- EGR sweep with passive pre-chamber using Co-Optima O30 fuel.
- Dilution tolerance (COV>5%) of passive PC limited to EGR 10%.
- Rapid flame development and shorter burn duration within dilution limit.



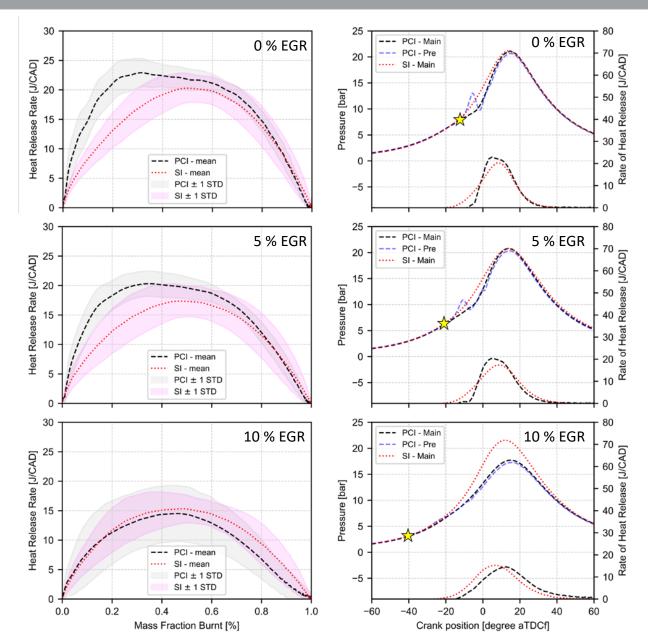


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- No pressure build-up in pre-chamber at 10 % EGR.



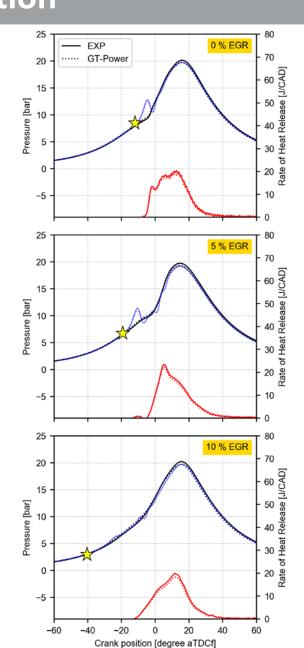
Technical Accomplishments – E.1.2.5, Rockstroh, ANL Pre-chamber assisted MM operation

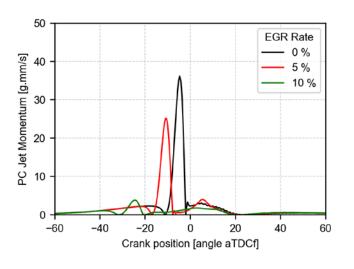


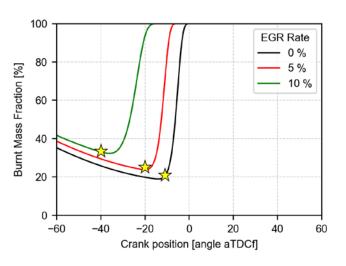
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- EGR sweep with passive pre-chamber using Co-Optima O30 fuel.
- Dilution tolerance (COV>5%) of passive PC limited to EGR 10%.
- Rapid flame development and shorter burn duration within dilution limit.
- No pressure build-up in pre-chamber at 10 % EGR.
- GT-Power model replicates pre-chamber and main chamber combustion.
- Pre-chamber jet momentum diminishes with dilution due to excessive burnt mass fraction.

Air-fuel supply system is expected to restore prechamber jet momentum and extend dilution tolerance

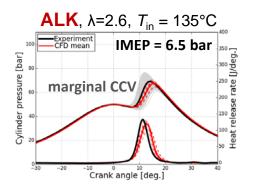


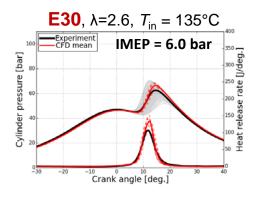


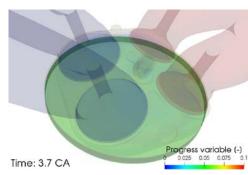


Technical Accomplishments – G.1.1.1, Scarcelli, ANL Fuel impacts simulated over the entire MM operating range









Objective: Simulate the full MM range (ACI → SACI → SI) in a GDI engine platform

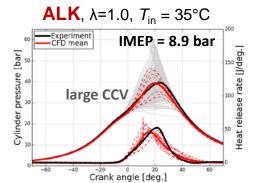
Low-load ACI operation

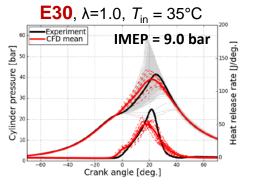


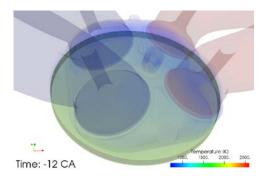
- RANS with MZ-WSR + G-equation validated for the full range of multi-mode combustion regimes, from ACI to SI operation, for two Co-Optima core fuels (ALK, E30).
- The simulations capture primary characteristics of combustion process for ACI (volumetric sequential auto-ignition) and SI (surface flame propagation) as shown in the movies below.
- Multi-cycle simulations exhibit experimentally comparable CCV trend for both distinct operation modes.



CFD model ready to evaluate ACI/SI transition and fuel effects







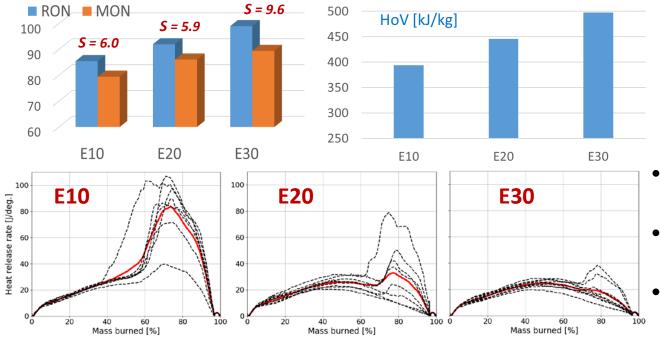
Technical Accomplishments – G.1.1.1, Scarcelli, ANL ACI/SI transition and fuel effects evaluated

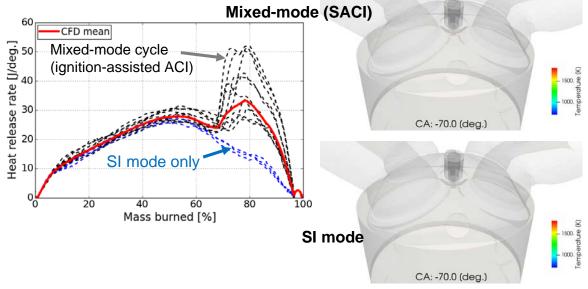


Objective: Simulate the full MM range (ACI \rightarrow SACI \rightarrow SI) in a GDI engine platform

<u>Test condition^{1,2)}</u>: **E30**, λ =1.75, T_{in} = 100°C, P_{in} = 85 kPa, ST = 57 CA bTDC, CR=12, IMEP=4.6 bar

- Virtual SACI test condition leveraged on-going mixed-mode studies in Co-Optima (PI: Sjoberg, SNL).
- Simulation captured ignition-assisted ACI in the ANL single-cylinder GDI engine. Strong deflagration wave may enhance the reactivity of end-gas state and promote auto-ignition.





- Simulated effect of ethanol blending level (% vol) on SACI mode at low loads.
- Laminar flame speed not much affected by ethanol blending (see backup slide). Much larger impact on RON/MON and HoV.
 - Lower ethanol blending enhances ACI mode at low loads. High ethanol content may be more beneficial at high load SACI.

Fuel effect on low load ACI/SI transition evaluated

Technical Accomplishments — G.1.1.1, Scarcelli, ANL CFD model built for pre-chamber (PC) assisted MM operation

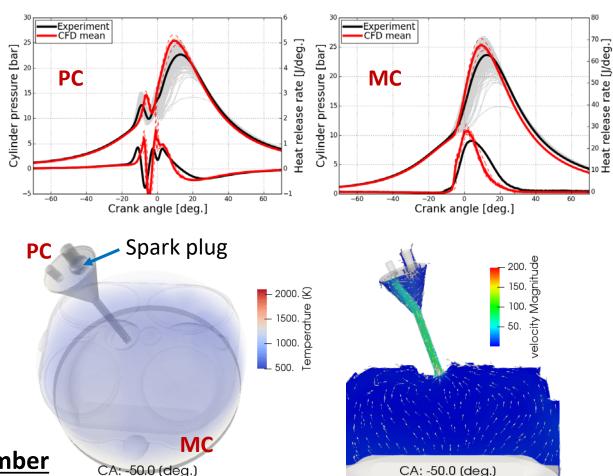


Objective: Evaluate the use of advanced ignition (prechamber, PC) strategies to enhance MM operation

- Preliminary simulation and validation of the CFD model adapted to study PC-assisted MM.
- Initial benchmark against stoichiometric, un-fueled (or passive) PC operation.
- Features of experimentally observed combustion process are moderately captured.
 - Turbulent flame jet ignition leading to fast burning rate and marginal CCV
- Improved agreement will require in-depth study of mass transfer between PC and MC.
- Future investigations will focus on PC-ACI → PCSI model validation and impact of fuel properties.

<u>CFD model ready to evaluate impact of pre-chamber ignition and fuel effects on multi-mode operation</u>

<u>Test condition</u>: ALK, λ =1.0, T_{in} = 35°C, P_{in} = 40 kPa, ST = 18 CA bTDC, passive (non-fueled) pre-chamber



PC: pre-chamber, MC: main-chamber

Technical Accomplishments — G.5.5, Edwards, ORNL

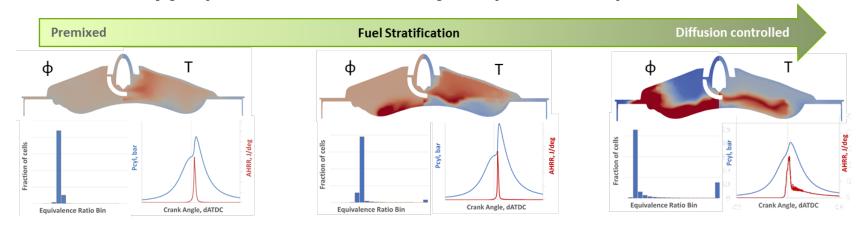




Objective: Develop and evaluate a flexible model to explore ACI sensitivity over full range of stratification

- Developed flexible CFD model for MM/ACI simulations
 - Based on stock boosted-SI architecture (Ford 1.6-L GDI) for MM operation
 - Piston modified to enable higher CRs
 - Multiple DI injection strategies with stock injector for fuel stratification
 - No spark in current efforts
- Demonstrated ability to capture full range of fuel stratification: HCCI => PPCI => MCCI
 - Engine/injector not well-suited for MCCI (pooling, high HC and soot) so not included in subsequent simulations
- Initial parameter sweeps performed for individual sensitivities and functionalities
 - Results used to refine parameter space and target sampling to regions of high sensitivity and high performance
 - Supported completion of FY19Q3 milestone

Model ready for production runs over refined parameter space



Moderate detail to enable rapid simulations

- CONVERGE v2.4
- ~725k cells
- 8-species E30 fuel surrogate
- E30 mechanism (138 species, 623 reactions)
- LLNL mechanism reduced by UConn
- RANS turbulence
- Walltime: ~18 hrs/cycle wall-time on 72 cores

Parameter	Initial Range	Refined Range
T intake	25 – 160 °C	25 – 275 °C
P intake	0.5 – 2 bar	0.5 – 3 bar
EGR%	0 – 60%	0 – 60%
gIMEP target	Up to 6 bar	Up to 5 bar
PM/DI ratio	HCCI (100% PM) PPCI (90–10% PM) MCCI (0% PM)	HCCI (100% PM) PPCI (90–10% PM)
DI SOI	-80 to +10 dATDC	-100 to +15 dATDC
CR	8 – 16	focus on 14

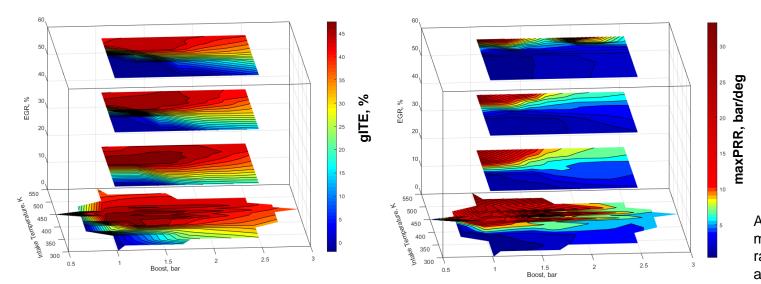
Technical Accomplishments – G.5.5, Edwards, ORNL Analyzing ACI cycle-to-cycle variability

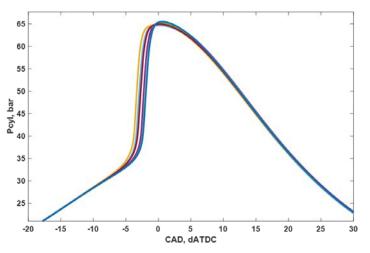


Objective: Perform production runs over full parameter space

- Completed refined multivariate study of operating parameter sensitivities
 - ~450 multi-cycle simulations
- Simulations capture limited cyclic variability (CCV) in ignition delay
 - CCV not severe enough to affect capture of global trends.
 - Most cases ran for 2-3 cycles. Future studies will simulate more cycles for improved statistics.
- CFD results are now being used to train low-order models with TASMANIAN for more rapid exploration of the parameter space
 - TASMANIAN = Toolkit for Adaptive Stochastic Modeling and Non-Intrusive Approximation.

Further analysis and additional simulations with parameterized fuel properties are ongoing





PPCI case showing predicted variability in ignition delay over 7 consecutive cycles

Along with automated mathematical analysis, manual survey using multivariate contour plots of portions of the parameter space enable rapid identification of key areas of interest for further study including areas with high performance or high sensitivity

Responses to Previous Year Reviewers' Comments



Reviewer: "The reviewer indicated that a good result of using the RCM instead of real engine conditions in order to determine boost requirements was achieved. The finding that RON and sensitivity do not fully capture fuel reactivity in ACI modes was certainly interesting to the reviewer and needs further work. As this result is aligned well with the Co-Optima goals, it is a good result. However, the reviewer expressed interest in knowing how significant the finding is and how representative it is when used in fuel blends. The reviewer asked if there are other competing effects that might wash out any difference in fuels, as is suggested in the analysis of alkylate and E-30 fuels.. The reviewer questioned how well the kinetic mechanisms are correlated to the RCM data shown.."

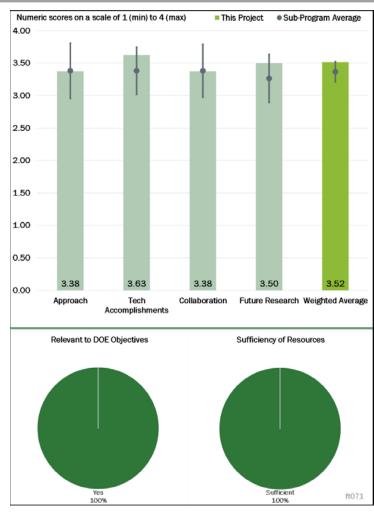
Response: We appreciate the feedback from the reviewer and the fact that they value the approach taken to characterize fuel autoignition behavior in a device with very well controlled environment. While we agree that the autoignition behavior in an engine is complicated by features such as thermal stratification, charge cooling, mixture concentration etc., we believe that it is important to try separate these, to conduct a true assessment of autoignition behavior. Detailed kinetic simulation is an indispensable tool for the development of ACI engines and kinetic modelling groups are continuously improving model and surrogate fuel formulations.

Reviewer: "What was unclear to the reviewer is if the CFD approach to capture the global trends across the full ACI spectrum includes all of the appropriate parameters in the appropriate range. It was unclear how these parameters were selected. In addition, it was unclear to the reviewer how these results will be incorporated into experimental efforts and how the timeline of these and other CFD efforts interact with the experimental work. The reviewer asked how well global trends can actually reflect ACI operation and what kind of accuracy is required in the models.

Response: The CFD task from ANL (PI: Scarcelli) is tightly connected to the corresponding ANL experimental task (PI: Rockstroh). CFD investigated the impact of fuel properties and engine parameters on ACI combustion in the same fashion as the experiments was carried out, and engine parameters were selected from engine experiments. Building a solid CFD model for fuel ACI/MM investigations allows generating a priori calculations on how fuel properties impact combustion that can be leveraged by experimentalists to test advanced fuels matching those properties.

Reviewer: "What was unclear to the reviewer is if the CFD approach to capture the global trends across the full ACI spectrum includes all of the appropriate parameters in the appropriate range. It was unclear how these parameters were selected."

Response: The initial parameter space was selected to include those parameters believed to significantly impact overall ACI performance. Additional factors that have lesser impact on global behavior are not initially considered but could be added later. Following the initial scoping study, parameter ranges were refined to ensure appropriate coverage of the operating space.



Scores and comments from 2019 Annual Merit Review Report ft071 MM: Auto-ignition in MM/ACI Combustion, Part 2

Collaborations



Extensive, interdisciplinary collaboration exists across the Co-Optima program

- DOE-funded research at National Laboratories, universities, and industry
- Input from stakeholders and advisory board
- Regular program reviews (AMR, AEC MOU)

Pacific Northwest National Laboratory Richard, WA Pacific Northwest National Laboratory Untermose, CA Pacific Northwest National Laboratory Universities National Renewable Energy Laboratory Augoring National Renewable Energy Laboratory Universities National Laboratory

G.5.5, Edwards, ORNL

- Convergent Science, Inc.
- LLNL (Pitz, et al.) Detailed kinetic mechanisms
- UConn (Lu) Reduced kinetic mechanisms
- ORNL (Sluder) Complimentary experiments on Ford GDI MCE
- ANL (Som, et al.) Integration of MCE, CFD, and vehicle systems modeling

E.1.2.5, Rockstroh, ANL

- Ford Support for engine modifications
- ANL (Goldsborough, et al.) Rapid compression machine (RCM) data
- ANL (Scarcelli) Complimentary CFD simulations

G.1.1.1, Scarcelli, ANL

- Convergent Science, Inc.
- LLNL (Pitz, et al.) Detailed kinetic mechanisms
- UConn (Lu) Reduced kinetic mechanisms
- ANL (Rockstroh) Complimentary experimental effort

Remaining Challenges and Barriers



Current efforts for these tasks address the following barriers and objectives outlined in the Co-Optima 3-year plan

E.1.2.5, Rockstroh, ANL

- Experimental investigation of fuel property effects on dilute stoichiometric engine operation with an active pre-chamber to be completed
- Characterize the potential of pre-chamber assisted compression ignition (PCACI) with Co-Optima core fuels
- Evaluate fuel octane and autoignition chemistry effects on PCACI combustion

G.1.1.1, Scarcelli, ANL

- Impact of fuel properties on the different modes (ACI, SACI, SI) in a MM engine is still unclear
- Most computational efforts study the effect of perturbing one or more specific properties, not the actual fuel
- Some fuels of interest require reduced kinetics to be simulated using CFD multi-dimensional solvers

G.5.5, Edwards, ORNL

- Assess fuel property impacts on engine efficiency, fuel economy and emissions
- Completion of sufficient number of CFD cases to accurately train low-order models. Number of cases needed depends on number of variables considered and sensitivity to those variables.

Proposed Future Research



E.1.2.5, Rockstroh, ANL

- Broaden study of the impact of fuel properties (SL, OI, ACI#, C/H, etc.) on both PCACI and PCFI operation, and identify desirable fuel properties for PC-assisted MM operation.
- Evaluate PC strategies (e.g. lean vs EGR dilution, PC fuel injection strategies) to maximize the efficiency of MM operation.

G.1.1.1, Scarcelli, ANL

- Complete validation of SACI model with limited fuel database including Co-Optima and HPF candidates.
- Expand the study of fuel impact on PC-assisted MM to a larger fuel database by varying surrogate blend components. Identify the most promising fuel (or properties) to enhance PC-assisted MM operation.

G.5.5, Edwards, ORNL

- Perform initial fuel property sweeps to evaluate MM/ACI individual sensitivities (FY20 Q4 milestone)
 - Parameterization of key thermophysical fuel properties (HoV, vapor pressure, etc.)
- FY21: Refine full parameter space
 - Prioritize, add, and/or eliminate parameters as appropriate
 - Perform multi-cycle production runs (expect 1000s of cases over full engine and fuel property parameter space)
 - Analysis and reporting

Summary



Relevance

• Delivering fundamental understanding of fuel property impacts on multi-mode operation to advance the development for improved fuels and engines to enable greater energy security, and reduced emissions.

Approach

• Engine experiments and simulations provide insight into how fuel properties affect SI/ACI multimode engine combustion

Technical Accomplishments

- Assessed compression history effects towards the implementation of constant volume ignition delay metrics for combustion phasing control, and evaluated uncertainties associated with ignition delay simulation and defining of thermodynamic states.
- Commissioned a pre-chamber ignition system to characterize pre-chamber assisted compression ignition (PCACI).
- Developed a multi-mode CFD model of a GDI engine to investigate SI/ACI, transition combustion modes and fuel effects.
- Implemented a CFD model of a pre-chamber ignition system to study fuel property effects on MM operation.
- Developed a flexible CFD engine model to assess fuel effects on MM operation and CCV under various operation conditions.

Collaboration and Coordination

- Co-Optima includes collaborative research funded by 2 DOE offices at 9 NLs, 20+ univ, and industry with strong industry engagement including industry-led external advisory board, monthly stakeholder phone calls, and annual stakeholder meeting
- Tasks: strong collaboration between lab teams and with industry and academia

Proposed Future Research*

Continuation of collaborative experimental and simulation efforts towards the development of improved fuel properties and engine
operating regimes.



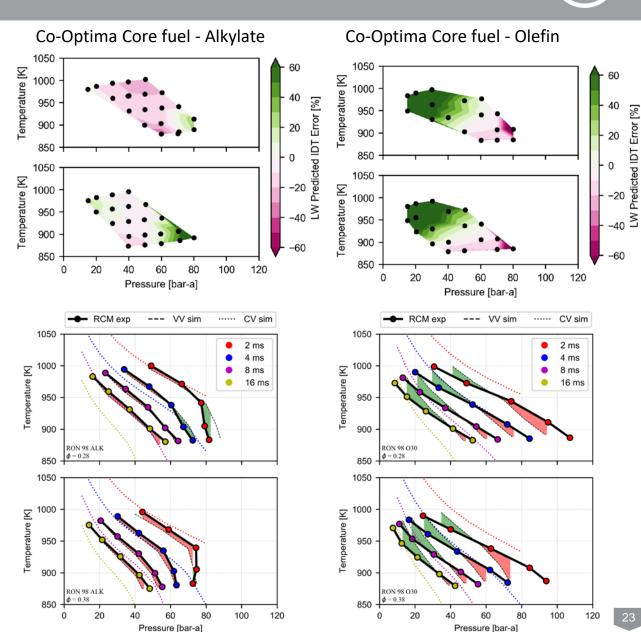
Technical Back-Up Slides

Technical Backup Slides – ANL Livengood&Wu assessment



Livengood&Wu (LW) integral vs SOC assessment

- Ignition delay measurements in ANL's Rapid Compression
 Machine (PI: Goldsborough) correlated against variable volume
 (VV) detailed kinetic simulations
- Compression history of the RCM measurements was assessed using the LW integral method and the error between the observed SOC and LW=1 was computed
- The kinetic mechanism replicates the RCM measurements quite well for Alkylate, while the Olefin fuel is captured less accurately
- Inaccuracies in estimating ignition delay carries over into the SOC prediction using LW – significant errors shown.

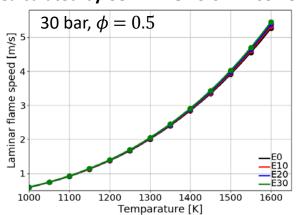


Technical Backup Slides – ANL CFD simulation setup

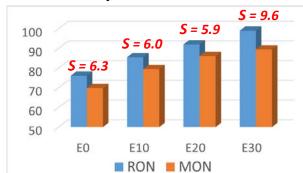


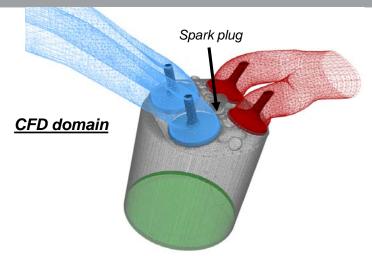
Software	CONVERGE CFD 2.4	
Combustion	Chemistry solution: CONVERGE SAGE solver Well stirred reactor with multi-zone model (ACI mode) Combined with level-set method (G-eqn) (SI & SACI mode)	
Chemistry	Co-Optima core fuel reduced (211 spc) mechanism developed by UConn	
Ignition	G source deposition	
Turbulence	Reynolds-Averaged Navier-Stokes (RANS) RNG k-e model	
Mesh resolution	 4 mm (base) through 0.5 mm by AMR (Adaptive Mesh Refinement) Fixed embedding: 0.25 mm (injector and valve seat regions) 0.125 mm in spark plug region 	
Discrete phase	 Eulerian-Lagrangian two-way coupling Composite species evaporation (Co-Optima fuel surrogates) 	

Calculated by CONVERGE 3.0 1-D solver



Calculated by CONVERGE 3.0 0-D solver





Engine platform	Ford single-cylinder GDI engine
Displacement	0.626 L
Compression ratio	15.3 (ACI), 12.7 (SI), 12 (SACI)
Engine speed	1500 rpm
Intake air temp.	100°C - 170°C (ACI) 35°C (SI)
Excess-air ratio (λ)	2.6 - 3.6 (ACI) 1.0 (SI) 1.75 (SACI)
Load	1.2 – 9.2 NMEP [bar]
Injection timing	-300° CA aTDC
CA50	12 CA aTDC (ACI)
Fuels	Co-Optima fuels (ALK & E30) for ACI, SI, SACI SACI: Ethanol blends with base gasoline